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MCNPX, VERSION 2.5.B

by

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1.0. INTRODUCTION

The MCNPX radiation transport code transports all particles at all energies. The latest release, MCNPX2.5.B is a superset of MCNP4C3, MCNPX2.3.0, and MCNPX2.4.0 plus a number of new capabilities.

1.1. Guarantee

MCNPX is guaranteed. We are so confident of the quality of MCNPX that we will pay $20 to the first person finding anything that does not meet or exceed the capabilities of MCNPX 2.3.0 and MCNP4C3. We also will pay a brand new $2 bill for any error in MCNPX that has been inherited from its constituent codes.[1]

1.2. Contents

1. Introduction
2. MCNPX 2.3.0 features new to MCNP users
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2.0. MCNPX 2.3.0 FEATURES NEW TO MCNP USERS

MCNPX includes all of the features and capabilities of MCNPX 2.3.0[2] (based on MCNP4B), which was recently released to RSICC. MCNPX features that will be new to MCNP users include:

- Physics for 34 particle types;
- High-energy physics above the tabular data range;
- Photonuclear physics (already in MCNP4C2);
- Neutron, proton, and photonuclear 150-MeV libraries and utilization;
- Mesh tallies (tally fluxes, heating, sources, etc., in a superimposed mesh);
- Radiography tallies;
- Secondary-particle production biasing; and

1 Cash Award Fine Print: Offer subject to cancellation or modification without notice. A bug is defined as an error in the source code that we choose to correct. We make awards even for the most trivial or insignificant problems, but not for proposed code enhancements or proposed extended capabilities. Awards given only to the first MCNPX user reporting a problem. Reported problems must be reproducible, and awards are paid when the correction is integrated into a forthcoming MCNPX version. We believe MCNPX and its predecessor codes are the most error-free and robust Monte Carlo radiation transport capabilities. We challenge you to find a bug!

2 Laurie S. Waters, Editor, "MCNPX User's Manual, Version 2.3.0," Los Alamos National Laboratory report LA-UR-02-2607 (April 2002).

- Autoconfiguration build system for compilation.

In particular, the mesh tallies enable users to plot source particle locations, fluxes, energy deposition, particle tracks, DXTRAN contributions, and other useful quantities on a superimposed tally grid. This capability is useful for all transport problems, not just high-energy problems.

3.0. MCNP4C3 FEATURES NEW TO MCNPX USERS

MCNPX includes all the features and capabilities of MCNP4C3. Until MCNPX2.4.0 (August 2002), MCNPX was based on MCNP4B (March 1997).[3] MCNPX now has all the capabilities of MCNP4C[45] (March 2000), MCNP4C2[6] (January 2001), and MCNP4C3[7] (April 2001). Initials of principal developers are shown in parentheses.[8] Principal among these features previously unavailable in MCNPX are

- PC enhancements: MCNPX is fully Linux and Windows capable (LLC/GWM);
- Easier geometry specification with macrobodies (LLC);
- Interactive geometry plotting (JSH);
- Improved variance reduction with the superimposed mesh weight window generator (TME/JAF/JSH);
- Superimposed mesh plotting (JSH);
- Delayed neutrons (CJW);
- Unresolved resonance range probability tables (LLC/RCL);
- Perturbations for material-dependent tallies (GWM/LLC/JSH);
- ENDF/B-VI extensions (MCW);
- Electron physics enhancements (upgrade to ITS3.0[9]) (KJA/HGH);
- Weight window enhancements (JSH/JAF); and
- Distributed memory multiprocessing (GWM).

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[3] J. F. Briesmeister, Ed., "MCNP—A General Monte Carlo N-Particle Transport Code—Version 4B," Los Alamos National Laboratory report LA-12625-M (March 1997).

[4] J. F. Briesmeister, Ed., "MCNP—A General Monte Carlo N-Particle Transport Code—Version 4C," Los Alamos National Laboratory report LA-13709-M (April 2000).

[5] J. S. Hendricks, "Advances in MCNP4C," Radiation Protection for Our National Priorities, Spokane, Washington, September 17–21, 2000, Los Alamos National Laboratory report LA-UR-00-2643 (2000).

[6] John S. Hendricks, "MCNP4C2," Los Alamos National Laboratory report LA-UR-01-858 (January 30, 2001).

[7] John S. Hendricks, "MCNP4C3," Los Alamos National Laboratory report LA-UR-01-2244 (April 13, 2001).

[8] Gregg W. McKinney (GWM), John S. Hendricks (JSH), Laurie S. Waters (LSW), Leland L. Carter (LLC), Franz X. Gallmeier (FXG), H. Grady Hughes (HGH), Richard E. Prael (REP), Stepan G. Mashnik (SJM), Arnold J. Sierk (AJS), Thomas J. Evans, Jeffrey A. Favorite, Christopher J. Werner, Robert C. Little, Morgan C. White, and Kenneth J. Adams.

[9] J. A. Halbleib, R. P. Kensek, T. A. Mehlhorn, G. D. Valdez, S. M. Seltzer, M. J. Berger, "ITS Version 3.0: The Integrated TIGER Series of Coupled Electron/Photon Monte Carlo Transport Codes," Sandia National Laboratories report SAND91-1634 (March 1992)

4.0. RECENT MCNPX FEATURES NEW TO BOTH MCNP AND MCNPX USERS

4.1. Summary of MCNPX 2.4.0 New Features

MCNPX has many new capabilities not found in either MCNP4C or MCNPX 2.3.0. The following features became available with MCNPX2.4.0,[10][11] which was released to the Radiation Safety Information and Computational Center (RSICC) in Oak Ridge, Tennessee, USA, on August 1, 2002. Details of these features are given in Section 4.3.

- FORTRAN 90 modularity and dynamic memory allocation (GWM);
- Distributed memory multiprocessing for the entire energy range of all particles (GWM);
- Repeated structures source path improvement (LLC/JSH);
- Default dose functions (LSW/JSH);
- Light-ion recoil (JSH);
- Enhanced color geometry plots (GWM/JSH);
- Photonuclear cross-section plots (JSH);
- Proton cross-section plots (JSH);
- Proton reaction multipliers with FM cards (JSH);
- Photonuclear reaction multipliers with FM cards (JSH/GWM);
- Some speedups (GWM/JSH);
- Logarithmic interpolation on input cards (JSH);
- Cosine bins that may be specified in degrees (JSH);
- Cosine bins may be specified for F2 flux tallies (JSH);
- Source particles that may be specified by descriptors (JSH);
- Pause command for tally and cross-section plots (JSH); and
- Correction of all known MCNPX and MCNP4C bugs/problems.

4.2. Summary of New Features After MCNPX 2.4.0

Since the release of MCNPX2.4.0, several new features and corrections have been added to MCNPX that are now available. These features are described in Section 4.4.

- CEM2k physics (SGM/AJS/FXG)
- Mix and Match (JSH)
- Positron Sources (HGH)
- Spontaneous Fission (JSH)
- Corrections (JSH)

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10 Laurie S. Waters, Ed., "MCNPX User's Manual Version 2.4.0," Los Alamos National Laboratory report, LA-CP-02-408 (September 2002).

11 MCNPX Team, "MCNPX, Version 2.4.0," Los Alamos National Laboratory report, LA-UR-02-5253 (August 2002).

4.3. Description of New MCNPX 2.4.0 Features

4.3.1. FORTRAN 90 Modularity and Dynamic Memory Allocation

The F90 conversion provides improvements in code modularity, standardization of functions such as timing across platforms, and compiler reliability. F90 will run more slowly on some systems. Specifically, we have eliminated equivalences as a means of dynamic storage allocation by using F90 pointers and allocable arrays. We have replaced most common calls with F90 modules. The code will compile in both free and fixed F90 formats.

MCNPX 2.4.0 can be modified by patches, and as much of the MCNP4C coding as possible has been preserved so that MCNP4C patches can be applied directly to MCNPX 2.4.0.

Continuing improvements in the F90 structure are ongoing, especially where they concern physics modules that have been brought into the code.

4.3.2. Distributed Memory Multiprocessing for the Entire Energy Range of All Particles

Parallel Virtual Machine (PVM) software can be used to run the entire MCNPX code in parallel. Fault tolerance and load balancing are available, and multiprocessing can be done across a network of heterogeneous platforms. Threading may be used for problems run in the table data region only.

4.3.3. Repeated Structures Source Path Improvement

Sources in repeated structures and lattices now may be specified with the same notation as tallies, and the paths are printed correctly in the output (see Section 5.2).

4.3.4. Default Dose Functions

Fourteen standard dose functions in United States (US) or international units may be applied to any tally without entering the tables on DE/DF cards (see Section 5.1).

4.3.5. Light-Ion Recoil

Neutrons and protons undergoing elastic scatter can cause light-ion targets (H, D, T, ^{3}He, and ^{4}He) to create particles (h, d, t, s, and a) that are banked for subsequent transport with the proper two-body kinematics (see Section 5.6.2).

4.3.6. Enhanced Color Geometry Plots

Sixty-four colors are now available. Cells may be colored by any cell-based quantity, not just material. Logarithmic shading of importances, weight windows, and summary information is automatic. Color-coded shading of mesh-based weight windows is available (see Section 5.7).

4.3.7. Photonuclear Cross-Section Plots
Photonuclear interaction cross sections and their secondary particle yields may now be plotted with the MCNPX cross-section plotter (see Section 5.8).

4.3.8. Proton Cross-Section Plots
Photonuclear interaction cross sections and their secondary particle yields may now be plotted with the MCNPX cross-section plotter (see Section 5.9).

4.3.9. Photonuclear Reaction Multipliers
Photonuclear cross sections and yields may be used to multiply fluxes and other tally quantities on FM tally cards. Now the production of various secondary particles and reactions such as photofission may be tallied (see Section 5.10).

4.3.10. Proton Reaction Multipliers
Proton cross sections and yields may be used to multiply fluxes and other tally quantities on FM tally cards (see Section 5.10).

4.3.11. Speedup
The increased generality and FORTRAN 90 conversion of MCNPX 2.4.k slow the code down by ~15%. However, in certain cases, some speedups have been added to make it faster than either MCNP4C3 or MCNPX 2.3.0, particularly for repeated structures/lattice plotting and few-particle MCNPX problems.

4.3.12. Logarithmic Interpolation

```
E4 1.e-5 10log 1.e5
```

is equivalent to

```
E4 1.e-5 .0001 .001 .01 .1 1 10 100 1000 10000   .
```

4.3.13. Cosine Specification in Degrees
Cosine bins may be specified in degrees for F1 current tallies. Cosine bins may now also be specified for F2 flux tallies (see Section 5.4).

4.3.14. Source Particles May Be Specified by Descriptors
Previously,

```
SDEF par = n,
```

where

```
n = 1,2,...,9,...  (numbers).
```

Now,

SDEF par = n,

where

n = n,p,...,h,... (character particle designators)

is optionally allowed (see Section 5.5).

4.3.15. Pause Command for Tally and Cross-Section Plots

The MCNPX geometry plot *PAUSE* command is now extended to tally and cross-section plots. When the word *PAUSE N* is put in a tally plotting COM input file, the picture will display for *N* seconds. If the command *PAUSE* (without the *N*) is in the COM file, then the display will hold until a key is struck.

4.4. Description of New Features after MCNPX 2.4.0 Features

4.4.1. CEM2k Physics

The CEM physics model has been upgraded from CEM95 to CEM2k and represents a significant physics improvement in MCNPX. CEM stands for Cascade-Exciton Model. A good reference is Stepan Mashnik's and Arnold Sierk's report LA-UR-01-5390 (2001): http://lib-www.lanl.gov/la-pubs/00818526.pdf. The following CEM2k description comes from the abstract of their report.

CEM2k incorporates new approximations for the elementary cross sections used in the cascade, using more precise values for nuclear masses and pairing energies, using corrected systematics for the level-density parameters and several other refinements. We have improved algorithms used in many subroutines, decreasing the computing time by up to a factor of 6 for heavy targets. Other improvements were motivated by new data on isotope production measured at GSI. CEM2k has a longer cascade state, less preequilibrium emission, and evaporation from more highly excited compound nuclei compared to earlier versions. CEM2k also has other improvements and allows us to better model neutron, radionuclide, and gas production in ATW spallation targets. The increased accuracy and predictive power of CEM2k are shown by several examples.

In addition, Franz Gallmeier has added a mix-and-match capability for photonuclear events that is the model for the full mix-and-match capability described in the next section. There is no user interface change for CEM2k, and old CEM95 calculations in MCNPX will not track.

4.4.2. Mix and Match

MCNPX can now mix and match physics models and data tables. It is now possible to specify some nuclides with models and other nuclides with data tables. It is also possible to use data tables up to their maximum energy value and then use models above that energy, even when the maximum table energy differs from nuclide to nuclide.[12]

The new mix-and-match capability is the default for MCNPX. To track previous results, it is necessary to specify the energy cutoff, E_c between the table and model regions. Models then will be used above E_c, even if table data go above E_c, and the highest values of the data tables will be used below E_c whenever the data table energies are less than E_c .

Here are several examples illustrating the significance of the new mix-and-match capability.

Consider neutrons interacting with a BGO detector. Bismuth will be modeled with tables up to the table maximum, 20 MeV, and then will use the physics models above. Germanium, for which there is no supported data table, will use physics models for its entire energy range. Oxygen will use the data table up to its maximum of 150 MeV and then use the physics models above.

Photonuclear reactions can now use physics models whenever above the data table range (150 MeV) or whenever the desired photonuclear data tables are unavailable. Note that photonuclear physics is modeled with the new CEM2k model, regardless of whether CEM is used for other particles. Use of photonuclear physics models is discouraged unless specifying CEM physics (*9th entry on LCA card).*

Proton calculations previously required using models for the entire energy range or a limited set of 42 data tables for the entire energy range. If just one nuclide was missing from a data table, then data tables could not be used at all. Now data tables can be used whenever they are available, and physics models will be used for the nuclides without data tables.

It is also possible to substitute different nuclides for different particle types using the new MXn:p card (see Section 5.11). For example, natural carbon and calcium can be used for neutrons and ^{12}C and ^{40}Ca can be used for protons and photonuclear reactions.

4.4.3. Positron Sources

Positron sources may now be specified: *SDEF par = -e* or *SDEF par = -3* . Note that positron physics in MCNPX, just as with MCNP and the Integrated Tiger Series (ITS), is

[12] John S. Hendricks, Gregg W. McKinney, and Franz X. Gallmeier, "Mix and Match with MCNPX," submitted to the American Nuclear Society Mathematics and Computation Topical Meeting, M&C 2003, Gatlinburg, TN (April 2003).

identical to electron physics except for positron annihilation. Electrons below the energy cutoff are terminated, whereas positrons below the energy cutoff produce annihilation photons. Also, the positrons have a positive charge and may be tallied using the FT card ELC option.

4.4.4. Spontaneous Fission Sources

Spontaneous fission may be specified as a source as: *SDEF par = SF* . Available nuclides are ^{238}Pu, ^{240}Pu, ^{242}Pu, ^{242}Cm, ^{244}Cm, and ^{252}Cf. When PAR=SF on the SDEF card, the following happens:

1. The source neutron is immediately lost to fission; nu-1 spontaneous fission neutrons are put in the bank and tracking continues with the vth spontaneous fission neutron.

2. Fission multiplicity (6h entry, PHYS:N card) is automatically turned on with the default width (fisnu = -1 = nuclide dependent) unless otherwise specified. Multiplicity and moments are printed in Print Table 117. Note: not all MCNPX versions presently have fission multiplicity available.

3. If more than one of the six allowed spontaneous fission nuclides is in a source cell, the fissioning nuclide will be chosen proportionately to the product of its atom fraction and the spontaneous fission yield for each nuclide. If no spontaneous fission nuclide is found in a specified source cell, the code exits with a bad trouble error, “spontaneous fission impossible.”

4. Once a spontaneous fission nuclide is chosen, the source particle (arbitrary energy = 2 MeV) is lost to fission and the spontaneous fission neutrons are generated as prompt neutrons. The number of spontaneous fission neutrons per source is sampled from the data by Ensslin. The energies are sampled from a Watt spectrum with parameters for spontaneous fission from appendix H.I.B of the MCNP manual.[13] Note, the ^{240}Pu Watt spectrum constants are used for ^{238}Pu.

4.4.5. Corrections and enhancements

- Proton light ion recoil fails for neutrons colliding with hydrogen in the free gas thermal energy range. Only applies when PHYS:N 6j 1 (7th entry on PHYS:N card set). A $20 award was given to Tom McLean, LANL, HSR-4. Documented in LANL internal memo D-10:JSH-02-101.
- XSEX3 no longer requires specification of multiple angle bins and will work if none are specified (NANG = 0) ,as requested by Flavien Lambert (REP).
- Correct printout of multigroup energies (JSH).

[13] Laurie S. Waters, Ed., “MCNPX User’s Manual Version 2.4.0,” Los Alamos National Laboratory report LA-CP-02-408 (September 2002).

- Prevent infinite loop if IXSDIR file missing (JSH).
- Mean free path not incremented in neutron model region (JSH).
- Collisions not counted for terminated particles in model region (JSH)
- Premature terminations from glando sampling (GWM).

5.0. USER INTERFACE FOR NEW MCNPX FEATURES

Section 4 provided a summary description of the new MCNPX features. This section now describes the user interface changes for the following subset of those features.

- Default dose functions: DFn;
- Repeated structures source specification: SDEF, SI;
- Logarithmic interpolation: Nlog;
- Expanded cosine specification: Cn;
- SDEF particle specification: SDEF par h;
- Energy straggling: PHYS:N 4j I;
- Light ion recoil: PHYS: N 6j R;
- Enhanced color geometry plots: COLOR;
- Photonuclear cross-section plots;
- Proton cross-section plots;
- Photonuclear and proton reaction multipliers: FM; and
- Mix and Match.

These features are described below and in the new MCNPX 2.4.0 manual.

5.1. Default Dose Functions

The MCNPX DFACT mesh tally capability has been expanded to provide standard dose conversions with the DE/DF cards.

Users may input a table as in MCNP/MCNPX (although the interpolation int = log or int = lin may now be placed anywhere). n = tally number, which implies particle type.

DEn E1 E2 int E3 ...
DFn F1 int F2 F3 ...

Or the following DF card is accepted:

DFn iu=j fac=F int ic=I ,

where the following entries are all optional.

iu = 1 = US units (rem/h)
iu = 2 = international units (sieverts/h)

Default: iu = 2 international units (sieverts/h)

fac = normalization factor for dose (acr is also accepted instead of fac).
fac = -1 = normalize results to Q = 20 by dividing the parametric form of Q [5.0+17.0*exp(-(ln(2E))*2/6)] from ICRP60 (1990), paragraph A12.
fac = -2 = apply LANSCE albatross response function.
Default: fac = 1.0.

int = "log" or "lin" results in "log" or "lin" interpolation of energy; the dose function is always linear. That is, "lin" results in "linlin" interpolation, and "log" results in "loglin" interpolation.

Default: for ic = 10, 40: log
for ic = 20,31-39: recommended analytic parameterization.

ic = i = standard dose function.

<u>i neutron dose function</u>
10 = ICRP-21 1971
20 = NCRP-38 1971, ANSI/ANS-6.1.1-1977
31 = ANSI/ANS-6.1.1-1991 (AP anterior-posterior)
32 = (PA posterior-anterior)
33 = (LAT side exposure)
34 = (ROT normal to length and rotationally symmetric)
40 = ICRP-74 1996 ambient dose equivalent

<u>i photon dose function</u>
10 = ICRP-21 1971
20 = Claiborne & Trubey, ANSI/ANS 6.1.1-1977
31 = ANSI/ANS-6.1.1-1991 [AP (anterior-posterior)]
32 = PA (posterior-anterior)
33 = (LAT side exposure)
34 = (ROT normal to length and rotationally symmetric)
35 = (ISO isotropic)

Default: ic = 10

Examples:

DF4

DF0 ic 40 iu 1 lin fac 123.4

```
DF1  iu=2 acr=-2 log ic=34
```

5.2. Repeated Structures Source Specifications

The CEL source specification for repeated structures geometries is now consistent with the tally specification. The old MCNP4C specification still works, but the new one is

```
sdef  cel=d3  pos=0 6 0 ext d1 rad d2 axs 0 1 0
si3 L (1<10[0 0 0]<11) (1<10[1 0 0]<11) (1<10[2 0 0]<11)
(1<10[0 1 0]<11) (1<10[1 1 0]<11) (1<10[2 1 0]<11)
```

All of the output prints now also are consistent.

5.3. Logarithmic Interpolation

Logarithmic interpolation is now allowed on input cards. It is similar to the IJMR interpolation of MCNP. For example,

```
e0     1.e-3 6log 1.e4
```

is interpreted as

```
e0  .001 .01 .1 1 10 100 1000 10000   .
```

5.4. Expanded Cosine Specification

Cosines may now be specified in degrees. They may also now be specified with flux tallies as

```
*C2  150 120 90 60 30 0   .
```

The * on the C2 card interprets cosines as in degrees. Entries must be such that the cosine is monotonically increasing.

5.5. SDEF Particle Specification

The source particle type now may be specified on the SDEF card by its symbol:

```
SDEF par=h
```

5.6. PHYS:n Changes

For neutrons, the fifth entry is the model/table energy cutoff (see new Print Table 101). In previous MCNPX versions, this was the third PHYS:N entry.

For particle types n > 2 (e,…, h,…), the fifth entry is the energy straggling (see Section 5.6.1).

For neutrons or protons, the seventh entry is the light-ion recoil control (see Section 5.6.2).

5.6.1. Energy Straggling (Particle Types n > 2)

Dick Prael's and Grady Hughes's energy-straggling model in MCNPX 2.2.6 and later is specified as follows.

PHYS:n 4j I (5th entry on PHYS:n card) ,

where

I = 0: Prael's new straggling model—an energy correction addressing stopping powers of charged particles (default)

= 1: continuous slowing down ionization model; and

= -1: straggling model used in MCNPX 2.2.4 and previous releases.

n = particle type:

for

n = N, entry I is the library energy cutoff (formerly the third entry);
n = P, entry I is unused; and
n = E, the straggling model control is the same as MCNPX 2.3.0 and MCNP4C3.

5.6.2. Light-Ion Recoil (Incident Neutrons and Protons only)

PHYS:n 6j R (seventh entry on PHYS:n card) ,

where

n = N or H (neutrons and protons only);

$0 < R \le 1$: number of light-ion particles (h, d, t, s, and a) to be created at each elastic scatter on light nuclei for H, D, T, ^{3}He, and ^{4}He. The ionization potential is accounted for, and the proper two-body kinematics is used (with neutron free-gas thermal treatment if appropriate) to bank the created particles with the proper energy and angle.

Auxiliary cards:

mode n h d t s a ,

where n and/or h is required to produce light-ion elastic recoil from either neutrons and/or protons and

h,d,t,s,a are required to produce any of these particles.

Note that protons colliding with hydrogen to produce more protons can produce an overwhelming number of protons; caution is required.

cut:N 2j 0 ,

where

N = h,d,t,s,a may be needed to produce low-energy elastic recoil ions. The default alpha (a) energy cutoff is 4 MeV; however, dropping the alpha cutoff to zero will result in the minimum energy cutoff for an alpha of 1 keV, thus enabling the creation of E > 1 keV alphas.

5.7. Enhanced Color Geometry Plots (D-10:JSH-2002-09)

The new plotting capabilities are accessible via either the interactive geometry plot capability or the command/prompt interface.

In the interactive capability, the “SCALES n” button has been moved up two lines (after the cursor) to make room for a larger “COLOR name” button. The default is “COLOR mat”, which colors problem cells by the program material number. This button must be clicked to get “COLOR off” (black and white) and then clicked again to color by whatever parameter is listed after the “Edit” button. For example, in the right margin, “cel” must be clicked, which will make the “Edit” quantity “cel”. Next, “COLOR” must be clicked so that it says “COLOR cel”; on the next plot, the color shades will be by program cell number.

In the command/prompt input mode, the label command must be set, such as

PLOT> label 0 1 rho;

the color command then must be set such as

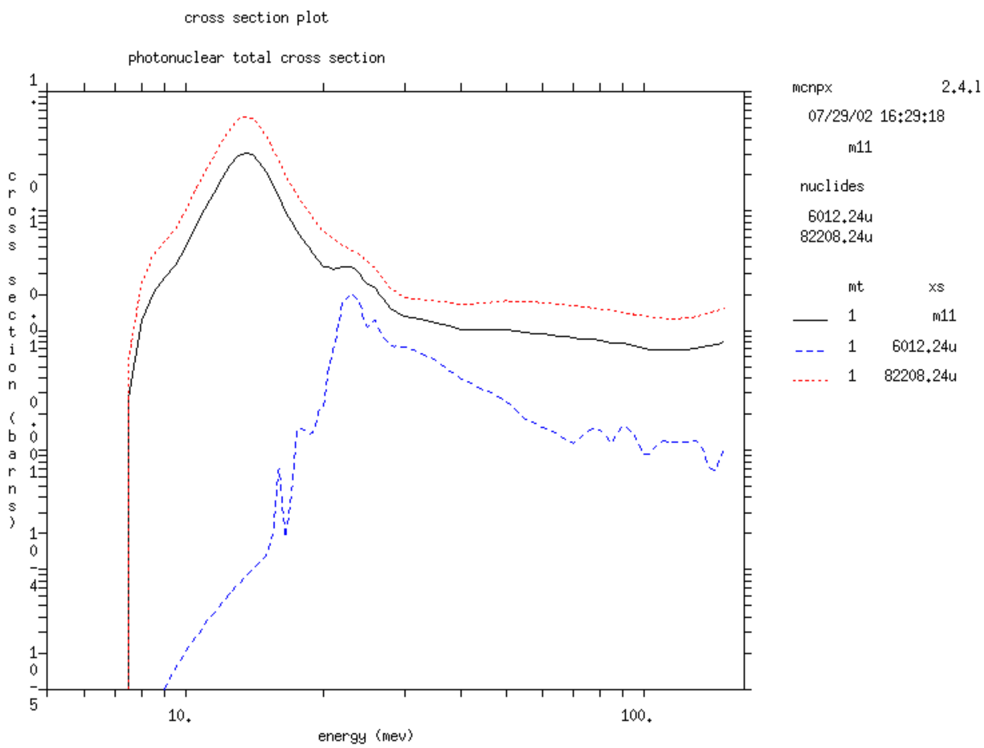
PLOT> color on

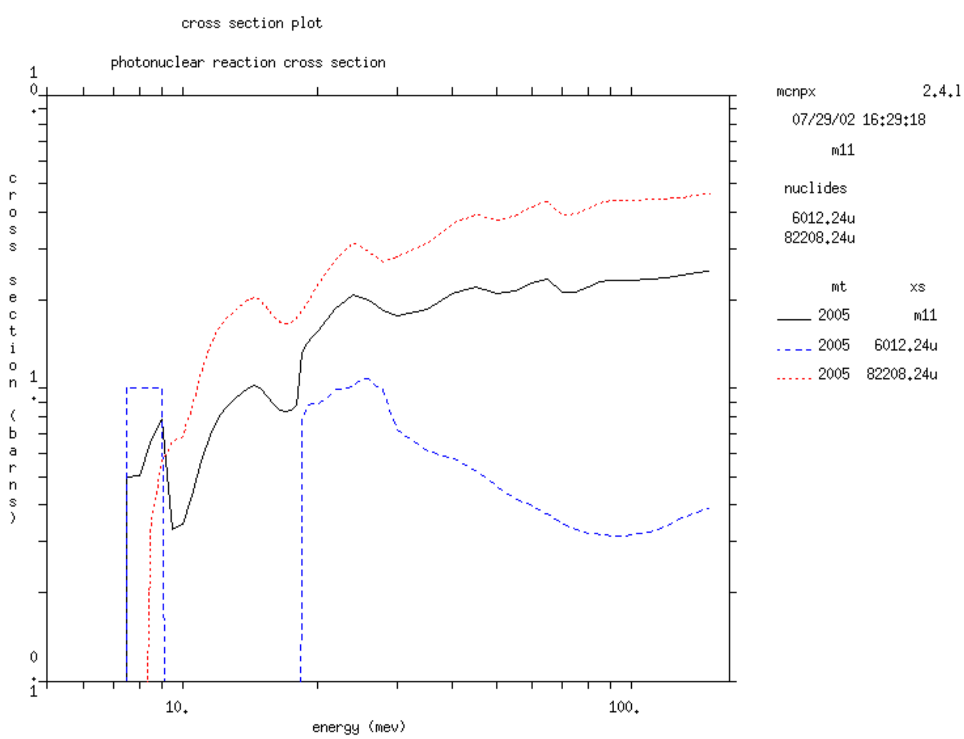
and the coloring will now be by rho, the atom density.

5.8. Photonuclear Cross-Section Plots (D-10:JSH-02-98)

Until now, only photon cross sections could be plotted in MCNPX. Photoatomic reaction numbers are all negative: -1 = incoherent, -2 = coherent, -3 = photoelectric, -4 = pair production, -5 = total, -6 = heating. For the MCNPX photonuclear cross-section plotting, the reaction numbers are all positive. The principal photonuclear cross sections are: 1 = total, 2 = nonelastic, 3 = elastic, 4 = heating, >4 = various reactions such as 18 = (γ,f). The photonuclear yields (multiplicities) for various secondary particles are specified by adding 1000 x the secondary particle number to the reaction number. For example, 31001 is the total yield of deuterons (particle type d = 31); 34001 is the total yield of alphas (particle type α = 34); 1018 is the total number of neutrons (particle type n = 1) from fission. To find out which reactions are available for a particular nuclide or material, enter an invalid reaction number, such as mt = 99 and MCNPX will list the available photonuclear reactions and the available yields such as 1018, 31018, 34018. Entering a bad nuclide, xs = 12345.67u, will cause MCNPX to list the available nuclides.

The following figures illustrate photonuclear cross-section plots for mt = 1 and mt = 2005.


cross section plot
photonuclear total cross section
mcnpx 2.4.1
07/29/02 16:29:18
m11
nuclides
6012.24u
82208.24u
mt xs
1 m11
1 6012.24u
1 82208.24u
cross section (barns)
energy (mev)
10.
100.


cross section plot
photonuclear reaction cross section
mcnpx 2.4.1
07/29/02 16:29:18
m11
nuclides
6012.24u
82208.24u
mt xs
2005 m11
2005 6012.24u
2005 82208.24u
cross section (barns)
energy (mev)
10.
100.

5.9. Proton Cross-Section Plots (D-10:JSH-02-98)

For proton cross-section plotting, the reaction numbers are similar to the neutron reaction numbers: all positive. The principal photonuclear cross sections are: ±1 = total, ±2 = nonelastic, ±3 = elastic, ±4 = heating, >4 = various reactions. On the LA150H proton library, the only available reaction is mt = 5 and its multiplicities, 1005, 9005, 31005, etc. The multiplicity reaction numbers for interaction reaction mt = 5 are 1005 for neutrons, n = 1, 9005 for protons, h = 9, 31005 for deuterons, d = 31, etc. To find out which reactions are available for a particular nuclide or material, enter an invalid reaction number, such as mt = 99, and MCNPX will list the available proton reactions and the available yields such as 1005, 32001, 34002, etc. The proton multiplicity, mt = 9001, 9004, 9005, etc., is generally available along with the total cross-section and heating number, mt = 1, mt = 4. Entering a bad nuclide, xs = 12345.67h, will cause MCNPX to list the available proton nuclides.

5.10. Photonuclear and Proton Reaction Multipliers (D-10:JSH-02-98)

Photonuclear and proton cross sections may be used in tally multipliers on the FM card. For example,

```
M102 92235 1 pnlib=27u
F2:P 1
FM2    (-1 102 18 1018)
```

It is always wise to plot the desired cross sections first to see if they are available with the expected reaction numbers in the data library. The tally multipliers treat the data the same as the data are treated in transport: the cross section at the lowest energy is extended down to E = 0 for protons with mt < 0; the cross section at the highest energy of the table is extended to E = ∞ for proton interaction cross sections with mt < 0 and for photonuclear interaction cross sections, mt < 1000. These extrapolations can be seen in the cross-section plots.

5.11. Mix-and-Match Nuclide Replacement (MX Card) (D-10:JSH-02-108)

A new input card is now available in MCNPX. It is a material substitution card, MX, that is an extension of, and replacement for, the MPN card for photonuclear data:

MXn:p zaid1 zaid2 ...

where n = material number of an Mn card that MUST precede the MXn card;
p = particle type (n, p, h)

zaidn = replacement nuclide for the nth nuclide on the Mn card.

Only particle types n, p, and h are allowed. No substitutions are allowed for photoatomic (p) and electron (e) data because those data sets are complete. The MXn:P card is an exact replacement of the MPNn card and specified photonuclear nuclide substitutions (library type u.) zaidn = 0 is allowed on MXn:P (photonuclear substitution) to specify no photonuclear data for a specific photoatomic reaction. zaidn = model is allowed on the MXn:N and MXn:H (neutron and proton substitution) to allow models to be mixed with tabular data. As an example, consider the following input file:

```
mode  n  h  p
phys:p  3j  1
m1        1002 1       1003.6 1     6012 1      20040   1      nlib .24c
mx1:n     j            model        6000        20000
mx1:h     model        1001         j           j
mpn1      6012         0            j           j
```

MCNPX will issue the following warnings:

```
warning. MPNn will soon be obsolete. use MXn:p instead.
warning. photonuclear za =  6012 different from nuclear za =  1002
warning. photonuclear za =     0 different from nuclear za =  1003
```

Note that models will be used for neutron tritium and proton deuterium; the MPN card still works but has a warning. The mixing and matching is summarized in new Print Table 101:

Print Table 101:

1particles and energy limits   print table 101

particle type			particle cutoff energy	maximum particle energy	smallest table maximum	largest table maximum	always use table below	always use model above
1	n	neutron	0.0000E+00	1.0000E+37	1.5000E+02	1.5000E+02	0.0000E+00	1.5000E+02
2	p	photon	1.0000E-03	1.0000E+02	1.0000E+05	1.0000E+05	1.0000E+05	1.0000E+05
9	h	proton	1.0000E+00	1.0000E+02	1.5000E+02	1.5000E+02	0.0000E+00	1.5000E+02

Notes: Because of the models, energy mix and match is now required from 0–150 MeV for both neutrons and protons.

6.0. FUTURE WORK.

- Cugnon Intranuclear Cascade (INC) model and Schmidt evaporation model.
- Special features for space applications.
- Weight windows variance reduction fully extended to physics models.
- Forced collisions for neutral particles extended to physics models.
- Secondary particle angle biasing for isotropic distributions.
- Improved high energy physics with the LAQGSM model.
- Multiple source particle types.
- Pulse height tallies with variance reduction.
- Neutral particle perturbation techniques extended to physics model region.
- Interactive tally and cross-section plotting.
- Detectors and DXTRAN for all neutral particles at all energy ranges.
- A capability to continue runs that write HTAPE files
- Integration of HTAPE tallies directly into MCNPX.
- Heavy ion tracking and interactions.

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8.0. BIBLIOGRAPHY

Code Manuals

Laurie S. Waters, Editor, "MCNPX User's Manual, Version 2.4.0," Los Alamos National Laboratory report, LA-CP-02-408 (September 2002).

Laurie S. Waters, Editor, "MCNPX User's Manual, Version 2.3.0," Los Alamos National Laboratory report, LA-UR-02-2607 (April 2002).

J. F. Briesmeister, Editor, "MCNP - A General Monte Carlo N-Particle Transport Code --- Version 4C," Los Alamos National Laboratory report, LA-13709-M (April 2000).

Laurie S. Waters, Editor, "MCNPX User's Manual - Version 2.1.5," Los Alamos National Laboratory report, TPO-E83-G-UG-X-00001 (November 14, 1999).

J. F. Briesmeister, Editor, "MCNP – A General Monte Carlo N-Particle Transport Code --- Version 4B," Los Alamos National Laboratory report, LA-12625-M (March 1997).

J. A. Halbleib, R. P. Kensek, T. A. Mehlhorn, G. D. Valdez, S. M. Seltzer, M. J. Berger, "ITS Version 3.0: The Integrated TIGER Series of Coupled Electron/Photon Monte Carlo Transport Codes," Sandia National Laboratories report SAND91-1634 (March 1992).

Code Version Release Announcements

MCNPX Team, "MCNPX, Version 2.4.0," Los Alamos National Laboratory report, LA-UR-02-5253 (August, 2002) http://lib-www.lanl.gov/documents/g/00783150.pdf.

John S. Hendricks, "MCNP4C2," Los Alamos National Laboratory report, LA-UR-01-858 (January 30, 2001).

John S. Hendricks, "MCNP4C3," Los Alamos National Laboratory report, LA-UR-01-2244 (April 13, 2001).

John S. Hendricks, "MCNP4C," Los Alamos National Laboratory memo, X-5:JSH-2000-30 (February 29, 2000).

John S. Hendricks, "MCNP4B," Los Alamos National Laboratory memo, XTM:JSH-97-13, (January 31, 1997).

Papers and Reports

John S. Hendricks, Gregg W. McKinney, Franz X. Gallmeier, "Mix and Match with MCNPX," submitted to the American Nuclear Society Mathematics and Computation Topical Meeting, M&C 2003, Gatlinburg, TN (April 2003).

J. S. Hendricks, G. W. McKinney, L. S. Waters, H. G. Hughes, E. C. Snow, ``New MCNPX Developments,'' LA-UR-02-2181, 12th Biennial Radiation Protection and Shielding Division Topical Meeting, Santa Fe, NM, American Nuclear Society, ISBN:8-89448-667-5, ANS Order No. 700293 (April 14–18, 2002).

Stepan G. Mashnik and Arnold J. Sierk, "Recent Developments of the Cascade-Exciton Model of Nuclear Reactions," International Conference on Nuclear Data for Science and Technology, October 7–12, 2001, Tsukuba, Japan. Los Alamos National Laboratory report LA-UR-01-5390 (2001), http://lib-www.lanl.gov/la-pubs/00818526.pdf.

E. C. Selcow, G. W. McKinney, T. E. Booth, J. F. Briesmeister, L. J. Cox, R. A. Forster, J. S. Hendricks, R. D. Mosteller, R. E. Prael, A. Sood, and S. W. White, "MCNP Capabilities at the Dawn of the 21st Century: Neutron-Gamma Applications,'' MC2000: International Conference on Advanced Monte Carlo for Radiation Physics, Particle Transport Simulation and Applications, Lisbon, Portugal (October 23–26, 2000), Los Alamos National Laboratory report LA-UR-00-5017.

J. S. Hendricks, K. J. Adams, T. E. Booth, J. F. Briesmeister, L. L. Carter, L. J. Cox, J. A. Favorite, R. A. Forster, G. W. McKinney, R. E. Prael, ``Present and Future Capabilities of MCNP,'' *Applied Radiation and Isotopes*, **53**, No. 4-5, 857-861, Elsevier Sciences, Ltd. (Netherlands), Pergamon Press, NY (October–November 2000).

J. S. Hendricks, "Advances in MCNP4C," Radiation Protection for Our National Priorities, Spokane, Washington (September 17–21, 2000) Los Alamos National Laboratory report LA-UR-00-2643.

G. W. McKinney, T. E. Booth, J. F. Briesmeister, L. J. Cox, R. A. Forster, J. S. Hendricks, R. D. Mosteller, R. E. Prael, A. Sood, ``MCNP Applications for the 21st Century,'' Proceedings of the 4th International Conference on Supercomputing in Nuclear Applications, Tokyo, Japan (September 4–7, 2000).

J. S. Hendricks, G. W. McKinney, L. J. Cox, ``Monte Carlo Advances for the Eolus ASCI Project,'' PHYSOR2000 International Topical Meeting on Advances in Reactor Physics and Mathematics and Computation, Pittsburgh, PA (May 7-11, 2000).

K. J. Adams, T. E. Booth, J. F. Briesmeister, L. L. Carter, J. D. Court, L. J. Cox, J. A. Favorite, R. A. Forster, J. S. Hendricks, G. W. McKinney, R. E. Prael, ``Present and Future Capabilities of MCNP,'' Fourth Topical Meeting on Industrial Radiation and

Radioisotope Measurement Applications (IRRMA 99), Raleigh, NC, page 38 (October 3–7, 1999).

H. G. Hughes, K. J. Adams, M. B. Chadwick, J. C. Comly, L. J. Cox, H. W. Egdorf, S. C. Frankle, J. S. Hendricks, R. C. Little, R. E. MacFarlane, S. G. Mashnik, R. E. Prael, A. J. Sierk, L. S. Waters, M. C. White, P. G. Young, Jr., F. Gallmeier, E. C. Snow, ``MCNPX for Neutron-Proton Transport,'' Proceedings of Mathematics and Computation, Reactor Physics, and Environmental Analysis in Nuclear Applications, Madrid, Spain, Vol. 2, p. 939–948 (September 1999).

Stepan G. Mashnik and Arnold J. Sierk, "Improved Cascade Exciton Model of Nuclear Reactions," proceedings of the Fourth Workshop on Simulating Accelerator Radiation Environments (SARE4), Knoxville, TN, September 14–16, 1998, T. A. Gabriel, Editor, ORNL, pp. 29–51 (1999).

H. G. Hughes, K. J. Adams, M. B. Chadwick, J. C. Comly, L. J. Cox, H. W. Egdorf, S. C. Frankle, F. X. Gallmeier, J. S. Hendricks, R. C. Little, R. E. MacFarlane, R. E. Prael, E. C. Snow, L. S. Waters, M. C. White, and P. G. Young, Jr., "Recent Developments in MCNPX," Proceedings of the Second International Topical Meeting On Nuclear Applications of Accelerator Technology, 281, Gatlinburg, TN, September 20-23, 1998.